

3-Amino-3-(naphthalen-1-yl)propanoic acid
100393-41-7 | DTXSID80377489

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.226

Global applicability domain: Inside

Local applicability domain index: 5.32e-01

Confidence level: 5.01e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Baclofen</div> <div>Measured: -0.960</div> <div>Predicted: 3.83e-02</div>	<div>Image not found</div> <div>Fenclonine</div> <div>Measured: -0.470</div> <div>Predicted: -0.770</div>
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